

## MODELLING OF HEAT AND MOISTURE TRANSFER IN CONCRETE AT HIGH TEMPERATURE

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**Abstract.** Moisture diffusion and related fluid pressures play a key role in cracking and spalling of concrete subject to high temperatures. This paper describes recent developments of a mode for moisture and heat transfer in porous materials, to be combined with an existing and well tested meso-mechanical model for concrete. Liquid and gas flows are formulated separately, yet later they can be combined in terms of a single variable,  $P_v$ . The material pore distribution curve is taken as the basis for developing a new physically-based desorption isotherm alternative to the traditional Bazant & Thonguthai's model. A simple academic example for temperatures between 27 and 800°C is presented to show the behaviour of the model.

### 1 INTRODUCTION

Two are the main mechanisms generally accepted to govern the development of cracking and fracture of concrete exposed to high temperature, for example in the case of fire. The first one is related to the incompatibility of thermal deformations between aggregates and cement paste, which may lead to stresses beyond elastic range. The second one corresponds to the water vapor pressure buildup in the pores, that may take place as the result of heat and water moisture transfer due to temperature and pressure gradients.

Original work of the group in this field was focusing on the first of those mechanisms [1,2] by means of a temperature-driven purely mechanical analysis of a meso-structural model which included cracking via zero-thickness interface elements [3,4]. The present paper describes the recent work on the study of the second of those mechanisms by means of a thermo-hygro model to analyse moisture movement and pore pressure build up as temperature increase.

Analysis of heat and moisture diffusion is generally based on the heat and mass water conservation equations combined with Fourier law (heat flow) and Fick's Law (moisture migration). These two diffusion processes may be considered uncoupled or coupled. The moisture diffusion analysis in turn may be represented with two independent variables (typically the two pressures of gas and water vapor or capillary pressure) [5,6], or be simplified to only one unknown variable [7]. For temperature below the critical point of water

(374.15°C), one must also distinguish between saturated and non-saturated (partially saturated) concrete; and in this case a constitutive equation for the pore state saturation may be needed. For higher temperature above the critical point, liquid water phase does not exist, and the equations of an ideal gas may be considered.

In the case of partial saturation, additional equations are needed to relate the water content of the pore system, to the partial pressure of the water vapor  $P_v$  and the capillary pressure  $P_c$ . These relations are a function of temperature  $T$ , and typically involve the degree of saturation  $S$  and the pore radius  $r$  distribution [8]. In the literature, these relations may take different forms; in Geotechnical literature the *water retention curves* relate the degree of saturation to the temperature and capillary pressure  $S=S(P_c, T)$ ; in materials science *sorption-desorption isotherms* relate water content to vapor pressure or relative humidity and temperature  $w=w(H, T)$ , where  $H= P_v/P_{sat}$  and the saturation pressure being a function of temperature  $P_{sat}=P_{sat}(T)$ .

One of the best known models is that of Bazant & Thonguthai's [7], which is based on a single primary unknown variable, the vapor pressure  $P_v$ , and proposes a set of phenomenological *isothermal desorption curves*  $w=w(P_v, T)$ . These curves have been used by many other authors, and in particular Tenchev [5] has modified the curves and extended the formulation to consider separate liquid water and water vapor pressures as independent primary variables.

Gawin & Schrefler [6], consider liquid water and water vapor separately in the mass transfer formulation, which are related through the saturation of liquid water, which are defined as a function of capillary pressure,  $S=S(P_c)$ , for a given temperature.

The present paper describes the new formulation developed to represent the thermal and moisture diffusion in concrete, which should eventually be coupled to the existing meso-mechanical model of the research group, in order to analyze the influence on the concrete damage and cracking due to high temperatures. Due to the many phenomena to be covered in the overall model, it has been established as a priority to try to maintain the representation of moisture diffusion with one single primary variable.

In a recent publication [9], a model was presented which consisted of a modification of the original formulation of Bazant and Tounghuthai's [7] which reduced the excessive pressures. However, although that model managed to reproduce qualitatively the pressure and water content profiles expected in basic 1-D, the formulation exhibited some significant shortcomings such as: (a) consideration of liquid and vapor water as a single phase for most purposes, (b) absence of physical basis for some of the assumptions and in particular the material pore structure was not taken into account, (c) sorption isotherm based on relative humidity  $H$ , concept that is not well defined after the critical point of water (374,15°C), (d) law that allowed the water content  $w$  to grow unlimitedly as the vapor pressure was increased, something not physical since water can only fill the available pore space. All these shortcomings have motivated the development of the new model presented in the following sections.

## 2 THERMAL AND MOISTURE TRANSFER MODEL

Same as in the previous model [9], the formulation may be separated into two parts: (a) desorption isotherm and (b) conservation equations, which are presented in the following

subsections.

## 2.1 Derivation of a desorption isotherm based on pore distribution and Kelvin equation.

One of the novel aspects of the model, for temperatures below the critical point of water, is the derivation of a desorption isotherm as the result of the combination of the pore distribution curve and some fundamental equations of thermodynamic equilibrium between water vapor and liquid water in the pores.

In the literature one can find different expressions for the degree of saturation of liquid water as a function of the capillary pressure [10-14]. Normally the empirical equations  $S=S(P_c)$  proposed are inaccurate when the saturation is close to zero since, in this field not much care is paid to the behavior at very low water content [8].

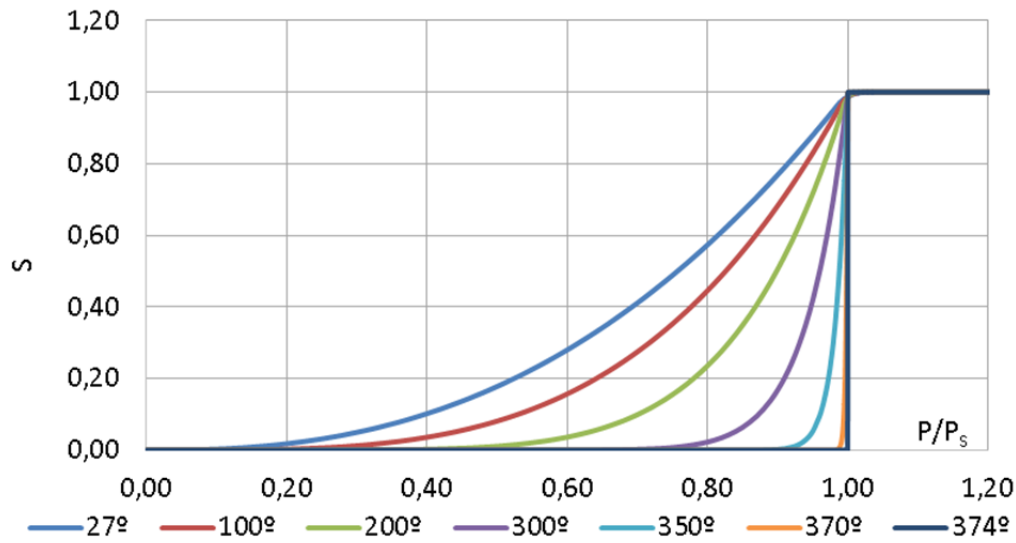
In the present study, the development starts from the pore size distribution curve  $S(r)$ , where  $S$  has the meaning of the fraction of the pore space which is contained in pores of diameter smaller or equal to  $r$ . This is complemented with the assumption that water will fill up first the smallest size pores then progressively larger pores. With this assumption, the curve  $S(r)$  can also be interpreted as giving the degree of saturation  $S$  for which the pore of radius  $r$  is partially filled (and all pores of smaller radii are totally filled, while all pores of radii larger than  $r$  are totally empty). Note that Kelvin's law supports this assumption in a partially saturated porous medium provided enough time has passed so that chemical equilibrium can be reached between water in the menisci and water vapor migrating from larger pores to smaller pores. For fast drying processes, larger pores are emptied first and therefore it seems also reasonable, while for fast wetting processes it may not be so certain to hold and strictly speaking it would require further investigation although here it has been assumed also for convenience.

Assuming an exponential-type expression for  $S(r)$ , and after combination with Laplace's and Kelvin's equations [8], one can obtain a power-type relation between  $S$  and  $P_v$  valid for temperatures below the critical point of water:

$$S = \left( \frac{P_v}{P_s} \right)^{\beta/m} \quad (1)$$

where  $P_s$  is the saturation pressure at the current temperature, and can be known using classical thermodynamic tables (Çengel & Turner, 2001) [15],  $\beta$  is a constant, and exponent  $m$  includes the effect of absolute temperature, the density of liquid water and the surface tension of water defined as an equation depending on temperature, as given in [16].

In figure 1, equation  $S=S(P_v, T)$  (1) is represented for a various values of temperature.



**Figure 1:** Evolution of the saturation degree in terms of the ratio  $P_V/P_s$  for different temperature values.

To obtain finally the total water content,  $w$ , must be related to  $S$  and  $P_v$ . For this purpose, total water content  $w$  may be decomposed as the sum of the liquid water,  $w_L$ , plus vapor water,  $w_V$ :

$$w = \underbrace{\phi S \rho_L}_{w_L} + \underbrace{\phi (1 - S) \rho_v}_{w_V} \quad (2)$$

where  $\phi$  is porosity;  $S$  is the degree of saturation,  $\rho_L$  is liquid water density [ $\text{Kg/m}^3$ ] which may be obtained from thermodynamic tables in terms of temperature (Çengel & Turner, 2001) [15], and  $\rho_v$  is the density of water vapor, which may be taken from the perfect gas equation:

$$\rho_v = \frac{P_v}{R_v T_a} \quad (3)$$

where  $R_v$  is the gas constant for water vapor [ $\text{J/Kg } ^\circ\text{K}$ ] and  $T_a$  is the absolute temperature.

Note that, expressions (1) and (3) replaced into (2) constitute a new physically-motivated desorption isotherm alternative to Bazant and Thongouthai's [7] for temperatures below the critical point of water. For temperatures above that point,  $S = 0$  and equation (3) simply becomes  $w = \phi \rho_v$ .

## 2.2 Conservation equations

Temperature distributions are obtained from separate thermal diffusion analysis (uncoupled), and only one pressure variable is considered to describe the water transfer process where the water dehydration is included.

The heat and water mass conservation equations may be expressed as:

$$\rho C \frac{\partial T}{\partial t} = -\text{div}(-k_T \text{grad} T) \quad (4)$$

$$\frac{\partial w}{\partial t} = -\text{div}(\bar{J}) + \frac{\partial w_d}{\partial t} \quad (5)$$

in which  $\rho$  and  $C$  are the mass density [ $\text{Kg/m}^3$ ] and heat capacity of concrete [ $\text{J/Kg } ^\circ\text{C}$ ],  $k_T$  is the heat conductivity [ $\text{J/Kg seg } ^\circ\text{C}$ ],  $w$  is the total mass of free water per  $\text{m}^3$  of concrete [ $\text{Kg/m}^3$ ];  $w_d$  [ $\text{Kg/m}^3$ ] is the mass of chemically bound water that is released to the pore as a result of the dehydration process (dehydration of the solids in cement paste as a result of heating); and  $\bar{J}$  is the total mass flow of water per unit area [ $\text{Kg/m}^2 \text{ seg}$ ].

Total mass flow of water,  $\bar{J}$ , may be also decomposed as the sum of the flow of liquid water,  $\bar{J}_L$ , plus the flow of vapor water,  $\bar{J}_V$ , both in [ $\text{Kg/m}^2 \text{ seg}$ ]:

$$\bar{J} = \bar{J}_L + \bar{J}_V \quad (6)$$

where, inserting Fick's laws for each of them, one obtains:

$$\bar{J}_L = -\phi S \rho_L \frac{k k_L}{\mu_L} \nabla P_L \quad (7)$$

$$\bar{J}_V = -\phi (1 - S) \frac{P_V}{R_v T_a} \frac{k k_V}{\mu_V} \nabla P_V \quad (8)$$

In the previous equations,  $\nabla$  indicates gradient,  $k$  represents concrete intrinsic permeability [ $\text{m}^2$ ];  $k_L$  and  $k_V$  are relative permeabilities of liquid water and water vapor, respectively,  $\mu_L$  and  $\mu_V$  are dynamic viscosities for liquid water and water vapor respectively en [ $\text{Kg/m}^2 \text{ seg}$ ]; and  $P_L$  and  $P_V$  correspond to the liquid pressure and vapor pressure, both in [ $\text{Kg/m}^2$ ]. Under the critical point of water, these two pressures are related by capillary pressure  $P_c$ :

$$P_L = P_V - P_c \quad (9)$$

Combining now equations (7), (8), (9) and Kelvin's equation, one obtains:

$$\begin{aligned} \bar{J} = & -\phi S \rho_L \frac{k k_L}{\mu_L} \left[ R_v \rho_L \ln \left( \frac{P_V}{P_s} \right) + R_v T_a \frac{\partial \rho_L}{\partial T} \ln \left( \frac{P_V}{P_s} \right) - R_v T_a \rho_L \frac{1}{P_s} \frac{\partial P_s}{\partial T} \right] \nabla T \\ & - \left[ \phi S \rho_L \frac{k k_L}{\mu_L} \left( 1 + R_v T_a \rho_L \frac{1}{P_V} \right) + \phi (1 - S) \frac{P_V}{R_v T_a} \frac{k k_V}{\mu_V} \right] \nabla P_V \end{aligned} \quad (10)$$

Note that thanks to assumptions made, only  $P_v$  shows up in this final equation.

The dehydration process is assumed to start at about  $105^\circ\text{C}$ , and the expression used is similar to that of Bazant and Thonguthai's [7]:

$$w_d = w_d^{105} f(T) \quad (11)$$

in which  $w_h^{105}$  is the hydrated water content at 105°C and  $f(T)$  is a function which represents the amount of water that is dehydrated when reaching higher temperature. Function  $f(T)$  is obtained by fitting experimental data of the weight loss measurements on heated concrete specimens, which can be obtained from the literature [17-19]. The expression used for  $f(T)$  is the following:

$$f(T) = 1 - \exp^{-q\left(\frac{T}{T_r}\right)^p} \quad (12)$$

where  $q$ ,  $p$  and  $T_r$  are constants fitting parameters which varies for different concretes and  $T$  represent the temperature.

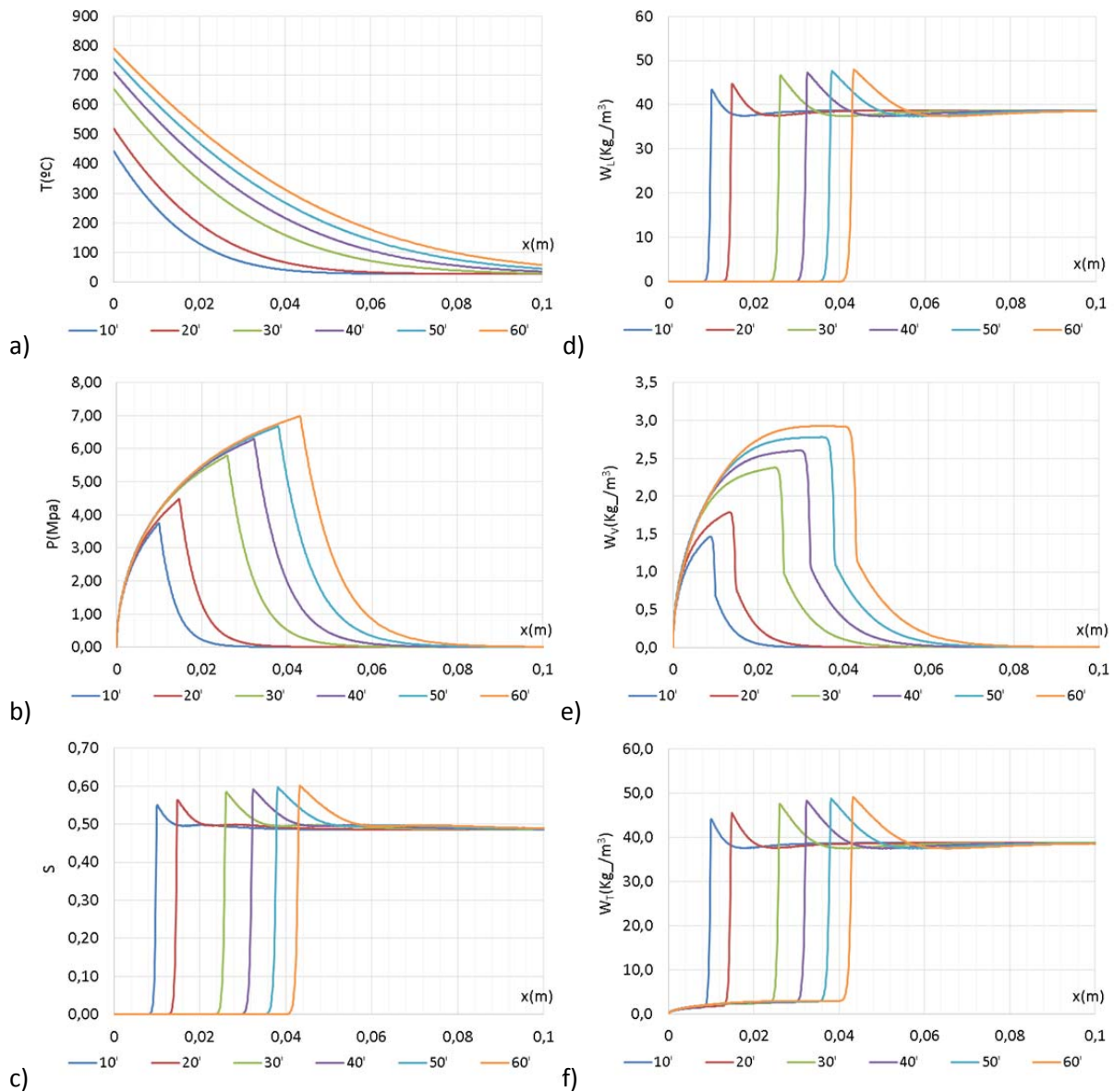
With equations (2), (10) and (11) the system is complete and equation (5) may be solved. The model described requires various additional parametric relations. Porosity  $\phi$  is defined as proposed in [5] in terms of initial porosity  $\phi_0$  and temperature. Intrinsic permeability of concrete  $k$  is also obtained using expression given in [5] in terms of initial intrinsic permeability  $k_0$  and porosity. Expressions for relative permeability of liquid water  $k_L$  and vapor  $k_V$  correspond to the ones used in [20]. Expressions for dynamic viscosity of liquid water  $\mu_L$  and vapor  $\mu_V$  in terms of parameters  $\mu_{V0}$  y  $\alpha_v$  and temperature have been taken from references [10] and [20].

### 3 RESULTS

The example of application presented in this section is a simplified version the one used in Tenchev *et. al.* (2001) [5] and Davie *et. al.* (2006) [20]. It consists of solving the 1D pressure distribution and water content in the direction perpendicular to the exposed surface, of a thick concrete wall. The numerical analysis is made on a long and narrow 2D FE domain of 20×0.2cm (horizontal×vertical), which is discretized with a single row of 730 linear rectangular elements and the left vertical end corresponds to the exposed surface.

Previous to the moisture calculation, temperature distributions are obtained from a separate thermal diffusion analysis, where the (left vertical) exposed edge is subject to temperature increments from 27 to 800°C according to the ISO 834 curve [21], condition which is applied *via* mixed Newman-Dirichlet boundary condition (heat flow proportional to the difference of the resulting surface temperature with the desired prescribed value, proportionality constant  $h$ ). Thermal flow is assumed null on the other three faces of the FE domain, and the initial temperature value is 27°C for all nodes of the mesh. The resulting temperature distribution is then applied as an input for the moisture diffusion analysis, with a constant vapor pressure value assumed prescribed on the (left vertical) exposed edge of the domain (of  $1,783\text{e}^{-3}$  MPa which corresponds to a relative humidity of 50% and 27°C), while moisture flow is assumed null on the other three faces. The initial vapor pressure value was  $2,67\text{e}^{-3}$  MPa for all nodes of the mesh, which corresponds a relative humidity of 75% at  $T_0 = 27^\circ\text{C}$ .

Thermal parameters used are:  $\rho = 2300 \text{ Kg/m}^3$ ;  $C = 1171 \text{ J/Kg}^\circ\text{C}$ ;  $k_T = 66 \text{ J/min m }^\circ\text{C}$  and the convective heat transfer coefficient,  $h = 6500 \text{ J/min m}^2 \text{ }^\circ\text{C}$ . For moisture diffusion analysis, the parameters used are:  $k_0 = 5\text{e}^{-17} \text{ m}^2$ ;  $\mu_{V0} = 1.475\text{e}^{-8} \text{ Kg min/ m}^2$ ;  $\alpha_v = 5.88\text{e}^{-11} \text{ Kg min/ m}^2 \text{ }^\circ\text{K}$ ;  $\beta = 2.5$ ;  $\phi_0 = 0.08$ ;  $R_v = 46.15 \text{ m}^\circ\text{K}$ ;  $T_0 = 27^\circ\text{C}$ ;  $\rho_L^0 = 1000 \text{ Kg/m}^3$ . The parameters to obtain the dehydration rate are:  $w_d^{105} = 60 \text{ Kg/m}^3$ ,  $T_r = 450$ ,  $q = 1$  and  $p = 3$ .



**Figure 2:** (a) Distribution of temperatures prescribed to the water content analysis; (b) vapor pressure; (c) saturation degree; (d) liquid water content; (e) vapor water content, (f) total water content as a function of the distance from the fire exposed edge for 10, 20, 30, 40, 50 and 60 minutes.

Figure 2 shows the curves of temperature prescribed  $T$  (2a), vapor pressure  $P_v$  (2b), saturation degree  $S$  (2c), resulting liquid water content  $w_L$  (2d), vapor water content  $w_v$  (2e) and total water content  $w$  (2f), as functions of  $x$  (depth in the concrete wall), for six different heating times of 10, 20, 30, 40, 50 and 60 minutes. Only the part of the mesh affected by the process is represented (from  $x=0$  to 0.1m), the rest remains in initial conditions. The results turn out qualitatively similar to those obtained in the literature, in which as the high temperatures penetrate the material, a front of low water content and high vapor pressure also moves into the material at around the location of the 250-300°C front.

In Figure 2, the zone of growing pressures can be seen (fig. 2b) to coincide with the zone of growing water vapor content (Fig. 2e). This is due to a faster rate of water evaporation than liquid water transport. Moreover, the zone where water vapor increases also coincides with the zone where liquid water is practically inexistent. The sudden drop in water vapor content right after the maximum value (Fig. 2e), coincides with the sudden transition from dry to saturated for similar times (Fig. 2d), all of which is dictated by the evolution of the saturation degree (Fig. 2c). For each time, the location of the maximum vapor pressure  $p$  marks pretty well the limit of the dry zone in corresponding  $S$  curve.

In Fig. 2d (liquid water distribution), one can clearly identify the four zones from left to right: a) a dry zone where liquid water has totally evaporated, b) a reduced zone of evaporation in which liquid water changes from its initial value ( $38 \text{ kg/m}^3$ ) to practically zero; c) a zone of growing liquid water content till a maximum over its initial value of  $38 \text{ kg/m}^3$  due to the flow towards the interior of the material due to the pressure gradient, with a condensation front when it reaches the interior zone at lower temperature (*moisture clog*); and d) the inner zone of material not affected by the process, where initial conditions remain.

#### 4 CONCLUDING REMARKS

The model described for moisture diffusion in concrete at high temperatures intends to be a physically-based model capable of representing the most essential aspects of moisture diffusion in concrete, while keeping the formulation simple enough (single-variable) so that eventually it can be implemented in the more general context of a meso-level mechanical model of concrete already developed and verified in a large variety of situations.

In previous work [9], a first attempt made was based on the isothermal sorption curves of Bazant and Thougouthai [7]. However some shortcomings were identified. The new formulation presented in this paper tries to overcome some of those limitations. Flow of water and vapor are initially considered as independent phenomena depending on their respective pressures, although later the use of Kelvin's equation brings the problem back to a single primary variable  $P_v$ . Desorption isotherms are not proposed phenomenologically, but come out as the result of the combination of a pore distribution curve and some fundamental laws such as Laplace and Kelvin's equations. The model uses the concept of  $P_s$  (and therefore relative humidity  $H$ ), only for temperatures below the critical point of water, and provides consistent transition to situations above that point, when only water vapor is present in the pores. Water content cannot grow beyond maximum material water capacity given by pore space. These and other advantages, make this model a sounder basis for incorporation into the complex meso-level model which is already under development.

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